POWGEN3: A High-Resolution Third-Generation Powder Diffractometer

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Abstract:

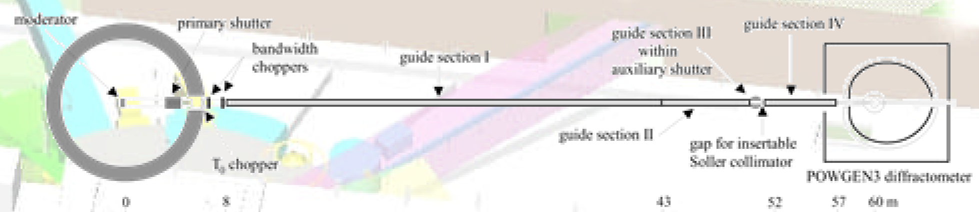
POWGEN3 is a fundamental departure from previous designs for a powder diffractometer at a spallation neutron source. POWGEN3 may be considered the world's first third-generation time-of-flight powder diffractometer. For the first time, a high-resolution powder diffractometer is able to take advantage of a high source repetition rate. Combined with a supermirror neutron guide system, POWGEN3 is a very efficient instrument. The high count rates thus achieved together with high-resolution characteristics present a big leap forward in performance over previous diffractometer designs. POWGEN3 will thus provide unprecedented opportunities for new science in the study of crystalline materials.

Third-Generation Concept:

First-generation time-of-flight powder neutron diffractometers grouped detectors into discrete banks around a few select scattering angles. To achieve a resonable d-spacing coverage in a single bank these instruments required a broad incident wavelength range.

Second-generation powder diffractometers expanded the angular coverage both in-plane and azimuthally about the beam, but still maintained the detector bank concept with data reduced effectively to a few scattering angles.

A **third-generation** concept, based on the idea put forward by Paolo Radaelli [1], is to use a narrow wavelength bandwidth and make use of wide angular coverage to collect data over all the *d*-spacings of interest. This narrow bandwidth method is well-matched to the 60-Hz repetition rate of the SNS source.



Supermirror Guide System:

The 49 m long supermirror neutron guide system, show in the schematic layout above, delivers x 15 (high-intensity mode) the neutron flux on sample (cf. no guide). The very high gain is achieved through using specially fabricated Ni-Ti multilayer mirrors and vertically tapering the final 14 m of the neutron guide. Intensity can be traded for improved resolution by inserting a newly developed solid-state silicon wafer Soller collimator [2] in the beam line. In this high-resolution mode the flux gain provided by the supermirror guide system is x 5.

Experiments:

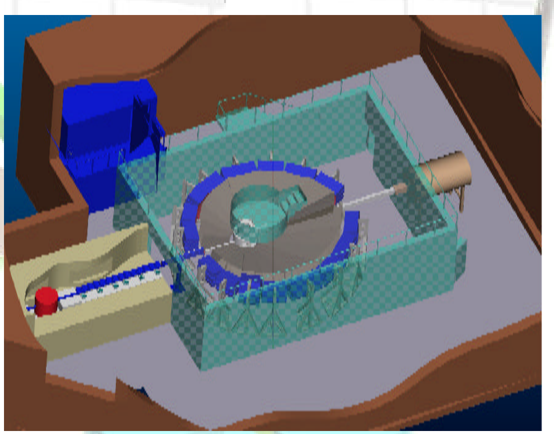
Parametric: investigate structural response of materials to changing applied conditions.

Static: elucidate magnetic and non-magnetic crystal structures with unprecendented accuracy and speed.

Materials:

Non-Magnetic: zeolite and AlPO frameworks, (fuel cell, battery and sensor) ionic conductors, thermoelectrics, ferroelectrics, molecule-hydrate cages, negative thermal expansion oxides, high-tech ceramics, minerals and pharmaceuticals.

Magnetic: high-T_c superconductors, collossal magnetoresistive perovskites, spintronics, metal-insulator transitions, charge and orbital ordering transitions, molecular magnets, frustrated & spin-glass magnets and heavy fermion phases.



Resolution Requirements & In-Plane Detector Locus:

Ideally, the resolution function for a powder diffractometer (intended for crystallographic as opposed to microstructural studies) should correlate with the density of Bragg reflections. For a cubic unit cell of dimension a_c the separation between adjacent reflections is

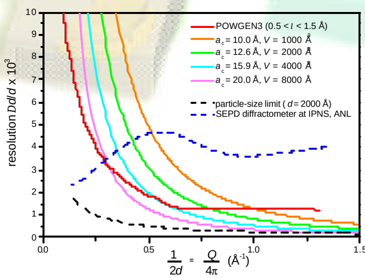
$$\frac{\Delta d}{d} = \frac{d^2}{2a_c^2}$$

For POWGEN3 to be considered a world class instrument, it will need to produce accurate crystal structures refinements up to $a_c \sim 20$ Å (cubic cell equivalent) complexity.

A number of analytical expressions for the detector locus have been evaluated by simulating realistic diffraction profiles and comparing the fitted resolution functions. The expression for an equiangular spiral:

$$r = Ae^{B\theta}$$

gave the best match to the desired resolution curve. A and B govern the size and curvature of the spiral, respectively.



[1] 'Extending the Domain of Time-of-Flight Powder Diffraction Techniques' P.G. Radaelli *The Fourteenth Meeting of the International Collaboration on Advanced Neutron Sources*, 1998, Vol. 2, pp. 159-168.

[2] 'Neutron Collimator with Rectangular Beam Profile' L.D. Cussen, P. Høghoj, I.S. Anderson, Nucl. Instr. and Meth. A 460 (2001) 374.

SNS Instrument Systems Argonne National Laboratory Oak Ridge National Laboratory

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